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Thermal transport in SiC nanostructures

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Abstract

SiC is a robust semiconductor material considered ideal for high-power application due to its material stability and large bulk thermal conductivity defined by the very fast phonons. In this paper, however, we show that both material-interface scattering and total-internal reflection significantly limit the SiC-nanostructure phonon transport and hence the heat dissipation in a typical device. For simplicity we focus on planar SiC nanostructures and calculate the thermal transport both parallel to the layers in a substrate/SiC/oxide heterostructure and across a SiC/metal gate or contact. We find that the phonon-interface scattering produces a heterostructure thermal conductivity significantly smaller than what is predicted in a traditional heat-transport calculation. We also document that the high-temperature heat flow across the metal/SiC interface is limited by total-internal reflection effects and maximizes with a small difference in the metal/SiC sound velocities.

Keywords: Phonon thermal transport, SiC nanostructure devices, Knudsen effect.

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1. Introduction

SiC is an exciting material with possible application in high-power devices but also posing interesting challenges for our understanding of the necessary heat dissipation. There are several SiC advantages, for example, structural robustness, presence of a native oxide (SiO_2), durability, and ability to grow high-mobility SiC layers on top of cheap Si substrates. The set of very fast phonons, the high purity, and the long phonon mean free path $l_{\rm mfp}$ also ensures a very large bulk thermal conductivity. On the one hand, this raises the promise for high-power device applications since it indicates an effective heat dissipation. On the other hand, the micron scale $l_{\rm mfp}$ invalidates the foundation of the traditional analysis based on the Fourier law of thermal transport. A finite-element approach that describes the local flow in terms of bulk values for the thermal conductivities breaks down because the phonon mean free path now approaches or exceeds typical feature sizes (thickness of conduction channel and oxide layers and distance between gates and contacts). We must instead turn to phonon-based calculations to describe SiC devices that represent a natural test case for developing an understanding of nanostructure thermal transport [1].

Figure 1 shows a structural schematics (upper panel) of a SiC device for which we document two phonon transport effects (lower panels) that significantly suppresses the heat dissipation. We observe that the thermal transport is completely dominated by the phonon dynamics even when discussing the conductance across a SiC/metal interface. For the phonon transmission problem we calculate the thermal conductance of SiC interfaces at room temperature, $\theta = 300$ K, and report the variation with general ratios of the material acoustic impedances and sound velocities. We find that this thermal conductance exhibits only a weak dependence on the ratio of acoustic impedances (which determines the long-wavelength phonon transmission) but a strong variation with the ratio of the material sound velocities (that define the total internal

reflection of phonons). In contrast to what is normally assumed, we argue that heat dissipation can be maximized by matching the sound velocities of the SiC and metal (or substrate).

We also document a phonon Knudsen effect that causes a significant suppression of the in-plane thermal conductivity for nanoscale layer thicknesses at room temperatures and even micronscale thicknesses at liquid-nitrogen temperatures, $\theta \approx 77$ K. At the same time we show that the traditional Fourier analysis breaks down in the description of such small structures and stress that shifting toward a phonon based description of thermal dissipation will become increasingly important with a continued downscaling.

2. Suppression of thermal transport across SiC/metal interfaces

Figure 2 illustrates the atomistic simple-cubic (SC) model adapted to estimate the finite-temperature thermal transport across the SiC/metal (or SiC/Si-substrate) interface. Both the phonon frequency ω and the in-plane momentum $q_{\|}$ (parallel to the interface) is conserved in this description of the phonon transmission. While approximative, our model description retains the important transport consequences of phonon total-internal reflection [2, 3].

This SC atomistic model has previously been used to calculate the phonon transmission and thermal transport in Si/Ge superlattices and heterostructures [2, 3]. Here we extend the SC model to describe the binary nature of the SiC material by choosing the SC volume $a_{\rm sc}^3$ to contain exactly one physical atom, but having an average atomic mass $M_{\rm SiC} = (M_{\rm Si} + M_{\rm C})/2$. The value of $a_{\rm sc} = 2.18$ Å corresponds to the physical (FCC) lattice constant $a_0 = 4.36$ Å of SiC [4]. Within each of the materials, these SC volumes are linked by force constants $F_{p,\,t;\,{\rm SiC}}$ with values which are fitted to the SiC sound velocities [4] $c_{l,t;\,{\rm SiC}} = a_{\rm sc}\sqrt{F_{p,t;\,{\rm SiC}}/M_{\rm SiC}}$, as expressed in the SC approximation [2]. In this model we also obtain acoustic impedances [3] $Z_{l,t;\,{\rm SiC}} = \sqrt{F_{p,t;\,{\rm SiC}}M_{\rm SiC}}/a_{\rm sc}^2$. We use

a corresponding notation ($F_{p,t;\,\mathrm{me}}, M_{\mathrm{me}}, \ldots$) to describe the SC phonon dynamics in the neighboring media 'me' (metal, Si, or general substrate). We assume for simplicity an identical lattice constant a_{sc} for both the SiC and the adjacent material, and we approximate the elastic coupling across the interface by $K_{p,t} \equiv \sqrt{F_{p,t;\,\mathrm{SiC}} F_{p,t;\,\mathrm{me}}}$.

Our calculation of the phonon conductance σ_{K} across the SiC/metal or SiC/substrate interface follows the approach and analysis of Ref. [3] to which we refer for a more detailed discussion. The modes in our SC model can be polarized either parallel ('p') or at right angles ('t') to the interface normal. In the following we focus on the description of the phonon dynamics and transmission of 'p'-polarized modes. The dynamics of a phonon moving in the SiC or neighboring media 'me' is then unique characterized by the conserved set $(\omega, q_{\|})$. We introduce frequencies $\Omega_{p,\,t;\,\mathrm{SiC\,(me)}} = 2\sqrt{F_{p,\,t;\,\mathrm{SiC\,(me)}}/M_{\mathrm{SiC\,(me)}}}$ and the (conserved) dimensionless measure $\alpha_{q_{\|}} = 2 - \cos(q_x a_{\mathrm{sc}}) - \cos(q_y a_{\mathrm{sc}})$ of the in-plane dynamics. The SC-phonon dispersion relation can be expressed

$$\Omega^2_{p;\,\mathrm{SiC(me)}} \left[1 - \cos(k_{\mathrm{SiC(me)}} a_{\mathrm{sc}})\right] = 2\omega^2 - \Omega^2_{t;\,\mathrm{SiC(me)}} \alpha_{q_{\|}} \tag{1}$$

and serve to establish the perpendicular momentum component $k_{\mathrm{SiC(me)}}$ of any phonon mode $(\omega, q_{\|})$ when moving in the SiC (and/or in the metal or substrate 'me').

We emphasize that this SC model description includes the affects of attenuation and of phonon total-internal reflection [2]. The attenuation (with associated thermal-transport suppression) arises because there is either insufficient or excess energy available for the perpendicular dynamics. A phonon with in-plane momentum $q_{\|} > 0$ that approaches from the typically softer 'me' side can be blocked from entering the hard SiC because the mode have too little energy to sustain the in-plane dynamics. Conversely, a mode $(\omega, q_{\|})$ which propagates in the SiC (having a real value of k_{SiC}) can have too much energy to enter the (softer) metal or substrate. In our SC model, both of these situations causes the dispersion relation (1) to yield an imaginary value of $k_{\mathrm{SiC(me)}}$, *i.e.*, the correct attenuated behavior on the SiC (me) side of the interface. At

elevated temperatures and with a finite separation in the sound velocities (material hardness) such total-internal reflection suppresses the thermal transport contribution from most of the available phase space [2, 3].

To quantify the resulting suppression of the conductance we calculate the SC estimates for the probability $T_K(\omega, q_\parallel)$ of phonon tunneling at general ω and $q_\parallel$ within our SC model. We extract $T_K(\omega, q_\parallel)$ by solving the Newton equation of motion for the phonon displacement $\eta_{q_\parallel;\,\mathrm{SiC}}(l \leq 0)$ and $\eta_{q_\parallel;\,\mathrm{me}}(s \geq 1)$ of the (atom-scale) SC elements located at the interface (here located between $l = 0$ and $s = 1$). Specifically, we consider then the reflection and transmission of an incoming SiC mode

$$\eta_{q_\parallel;\,\mathrm{SiC}}(l \leq 0) = e^{ik_{\mathrm{SiC}}a_{\mathrm{sc}}l} + A\, e^{-ik_{\mathrm{SiC}}a_{\mathrm{sc}}l} \tag{2}$$

$$\eta_{q_\parallel;\,\mathrm{me}}(s \geq 1) = B\, e^{ik_{\mathrm{me}}a_{\mathrm{sc}}s}, \tag{3}$$

and solve the harmonic equation

$$\begin{aligned}\eta_{q_\parallel;\,\mathrm{me}}(s=1)\ \left(2\omega^2 - \Omega^2_{t,\,\mathrm{me}}\alpha_{q_\parallel}\right)/2 &= \frac{F_{p;\,\mathrm{me}}}{M_{\mathrm{me}}}\left[\eta_{q_\parallel;\,\mathrm{me}}(s=2) - \eta_{q_\parallel;\,\mathrm{me}}(s=1)\right] \\ &+ \frac{K_p}{M_{\mathrm{me}}}\left[\eta_{q_\parallel;\,\mathrm{me}}(s=1) - \eta_{q_\parallel;\,\mathrm{SiC}}(l=0)\right].\end{aligned} \tag{4}$$

The tunneling vanishes, of course, exactly when there is attenuation on either sides of the interface; in the case when both k_{SiC} and k_{me} are real, we determine the tunneling probability

$$T_K(\omega;\, \alpha_{q_\parallel}) = 1 - |A|^2 \tag{5}$$

and hence obtain a description of the transport contribution at general $(\omega, q_\parallel)$.

We calculate the finite-temperature thermal conductance across the SiC/Metal interface by use of the formal result [5, 3]:

$$\sigma_K = \sum_{\mathrm{modes}} \int \frac{d^2q_\parallel}{(2\pi)^2}\left[\int \frac{d\omega}{2\pi}\,\hbar\omega\, T_K(\omega;\, q_\parallel)\left(\frac{\partial N_0}{\partial\theta}\right)\right] \tag{6}$$

The 'free' interface thermal conductance σ_0 that describe the phonon transmission across a SiC/SiC interfaces (for example, between the doped SiC substrate and the

undoped SiC transport channel) serves as a natural reference. We typically have the situation $\sigma_K(\theta) \ll \sigma_0(\theta)$ at finite temperatures [3] (for example, above the liquid-nitrogen temperature).

Figure 3 shows the results for the thermal conductance, σ_K, calculated at $\theta = 300$ K for a general SiC/metal or SiC/substrate interface within the SC model description. The plot reports a dramatic variation of σ_K as a function of the ratio of sound velocities $c_{\rm me}/c_{\rm SiC}$ and a much weaker dependence on the ratio of acoustic impedances $Z_{\rm me}/Z_{\rm SiC}$. Inserting the value for these ratios from Table I, the figure also documents that the typical SiC/metal and the SiC/Si interface at $\theta = 300$ K causes a dramatic suppression of the thermal conductance (when compared to the free conductance σ_0 value given by $c_{\rm me}/c_{\rm SiC} = Z_{\rm me}/Z_{\rm SiC} \equiv 1$). The study identify the need for further improving our understanding of the thermal coupling at such interfaces.

We also stress that this suppression of $\sigma_{\rm K}$ is qualitatively and quantitatively very different from the traditional conductance variation in low-temperature Kapitza effect. In the low-temperature regime the transmission is given by classical acoustics and hence exclusively defined by the ratio $Z_{\rm me}/Z_{\rm SiC}$. In the present finite-temperature regime it is instead the total-internal phonon reflection and hence $c_{\rm me}/c_{\rm SiC}$ that specifies the dominant thermal-conductance variation. In general the contact region between SiC and metals possesses a complex structure. Our calculation of the σ_K variation assumes a perfect junction between the SiC and the metal or Si substrate, rests on a simplified description of the characteristic phonon modes, and can thus only provide an approximative description. Nevertheless, our results strongly indicates that it is the difference in sound velocities rather than (as often assumed) the ratio of acoustic impedances which should be matched to maximize the high-temperature thermal transport out from a SiC power devices at contacts, gates, and cooling fringes.

3. Suppression of the thermal transport in SiC layers

We calculate the phonon Knudsen effect on the in-plane thermal transport by solving the linearized Boltzmann transport equation (l-BTE) in the relaxation-time approximation [6]. We consider a layer of thickness $d_{\rm layer}$ in which a small thermal gradient, $\nabla\theta \| x$, induces a change δN from the equilibrium phonon distribution $N_0 = 1/(e^{\hbar\omega/k_B\theta} - 1)$. The upper, lower materials boundaries are placed at $z_{>,<} = \pm d_{\rm layer}/2$ and we here use $q_z/q_\parallel$ to denote the component of the total phonon momentum, q, that is perpendicular to the layers/parallel to the in-plane temperature gradient $\nabla\theta$, respectively[2]. The bulk phonon mean free path, $l_{\rm mfp} = \mathbf{v}_q\tau_q$, is given by a product of the phonon group velocity and the (bulk) relaxation time. We assume, for simplicity, that $l_{\rm mfp}$ is independent of the mode and momentum and we fit $l_{\rm mfp}$ against measurements of the bulk-SiC thermal conductivity [7]. Solving then the l-BTE

$$\left\{\frac{q_z}{q}\frac{\partial}{\partial z} + \frac{1}{l_{\rm mfp}}\right\}\delta N = -\frac{1}{q}\left(\frac{\partial N_0}{\partial\theta}\right)\left(q_\parallel\,|\nabla\theta|\right), \tag{7}$$

in the absence and presence of the first term, we obtain and compare the distribution changes, $\delta N_{\rm bulk}$ and

$$\delta N_{\rm layer} = \delta N_{\rm Bulk}\left(1 - h_{q_z}(z,\, p_+,\, p_-)\right). \tag{8}$$

These distribution changes, in turn, determine the phonon thermal conductivity

$$\kappa_{\rm bulk,layer} = -(\nabla\theta)^{-1}\sum_{\rm modes}\int\frac{dq_\parallel}{(2\pi)}\int\frac{dq_z}{(2\pi)}\int\frac{dq_y}{(2\pi)}\hbar\omega_q\mathbf{v}_q\;\delta N_{\rm bulk,layer} \tag{9}$$

in the bulk and in the layered structure, respectively.

The interface scattering causes a suppression

$$h_{q_z}(z,\, p_+,\, p_-) = \sum_{\xi=>,<}\phi^\xi_{q_z}(p_+,\, p_-)e^{-|z-z_\xi|/\{l_{\rm mfp}(|q_\perp|/q)\}} \tag{10}$$

which depends on the fraction of specular $p_{+(-)}$ and diffusive $1-p_{+(-)}$ scattering at the upper (lower) material boundary. We determine the amplitudes $\phi^{>,<}_{q_z}$ of this variation

[2]The other in-plane momentum component is denoted q_y; we seek to keep a consistent notation between the two calculations although the direction of the temperature gradient differs.

from an analysis of the phonon scattering at the two interfaces, $z_{>,<} = \pm d_{\rm layer}/2$, following Refs. [7, 8, 9]. Specifically, for phonons that travel toward $z_> = d/2$ (with perpendicular momentum $q_z > 0$), the appropriate boundary condition for specular scattering is $\delta N(\Omega,\, q_z) \equiv \delta N(\Omega,\, -q_z)$, while the corresponding boundary condition for diffusive scattering is $\delta N(\Omega,\, q_z < 0) \equiv 0$. A similar treatment yields the boundary conditions at the lower interface, $z_<$, and an approach to determine the full variation of the suppression (10) by interface scattering.

We introduce $\overline{p} = (p_+ + p_-)/2$ and $\hat{p} = \sqrt{p_+ p_-}$ and express the resulting phonon Knudsen effect

$$\frac{\kappa_{\rm layer}}{\kappa_{\rm Bulk}}(\eta,\, p_+,\, p_-) = 1 - \frac{3}{8\eta}\left\{(1-\bar{p}) - 4\sum_{j=1}^{\infty} Q(j,\, \eta,\, \bar{p},\, \hat{p})\right\} \tag{11}$$

using special functions

$$Q(j,\, \eta,\, \bar{p},\, \hat{p}) = (\hat{p}^2 - 2\bar{p} + 1)\hat{p}^{j-1} D(j\eta) + (\bar{p} - \hat{p})(\hat{p}+1)^2 \hat{p}^{2(j-1)} D(2j\eta) \tag{12}$$

and

$$D(a\eta) \equiv \frac{1}{4}\left(1 - 5\frac{(a\eta)}{3} - \frac{(a\eta)^2}{6} + \frac{(a\eta)^3}{6}\right) e^{-a\eta} + \frac{1}{2}\left((a\eta)^2 - \frac{(a\eta)^4}{12}\right)\int_\eta^\infty dk\, \frac{e^{-ak}}{k}. \tag{13}$$

The analytical result extends earlier results [7, 9] and permits an efficient evaluation in the case where the degree of specular and diffusive scattering differs at the upper and lower boundary. The result (13) describes, in particular, the case when a thin (undoped) SiC transport channel is located below an oxide ($p_+ = 0$) and on top of a doped SiC substrate ($p_- \to 1$) or on a Si substrate ($0 < p_- < 1$, depending on the quality of the interface).

Figure 4 documents the significant phonon Knudsen effect caused by the interface scattering in two typical structures (inserts) at two different temperatures. The figure shows the variation in the effective thermal conductivity $\kappa_{\rm eff}$ evaluated as the weighted average of the (interface-limited) thermal conductivities describing the (finite) oxide,

(finite) SiC and (finite) Si-substrate layers. The figure documents that the Knudsen effects causes a very significant suppression of the thermal transport even up to hundreds of nanometers (micrometers) in the room (liquid-nitrogen) temperature cases.

Figure 4 further documents that calculations based on the traditional approach using Fourier law of heat conductions is inadequate due to the micron-scale phonon mean free path. The panels compares calculations with such a finite-element type description (dotted curves) against the present phonon-based transport calculations assuming both diffusive (solid curves) and specular (dashed curves) scattering at the SiC/Si-substrate interface. We find that the traditional approach completely breaks down at lower temperatures, and that moving to phonon-based calculations of thermal transport is essential for quantitative discussions of heat dissipation at room temperatures.

4. Conclusions

In this paper we have documented significant suppressions of the thermal transport both across a SiC/metal or SiC/substrate interfaces and within the SiC layer between a top oxide and the substrate. For the room-temperature thermal conductance we find that it is the ratio of material sound velocities, rather than of the acoustic impedances, which should be adjusted to maximize the thermal transport. For the thermal transport in a layered structure we further documented that interface scattering causes a significant suppression for nanoscale (micronscale) layer thicknesses at room (liquid-nitrogen) temperatures. Neither of these heat-transport effects can be addressed within the traditional description of heat transport based on the Fourier law. We conclude that the introduction of multiple interfaces and/or continued reduction of the thickness of the substrate or the conduction channels has adverse effects on the overall device heat dissipation. The ongoing quest for miniaturization motivates a shift toward phonon-based calculations of the thermal transport in nanostructure devices.

5. Acknowledgment

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TABLES AND TABLE CAPTIONS

Table 1: Materials properties and model parameters for the calculation of the room-temperature thermal transport across SiC/metal and/or SiC/Si interfaces.

	a_0 Å	M a.m.u	a_{sc} Å	c_l (m/s)	c_t (m/s)	$\left(\frac{Z_{\mathrm{me}}}{Z_{\mathrm{SiC}}}\right)_l$	$\left(\frac{Z_{\mathrm{me}}}{Z_{\mathrm{SiC}}}\right)_t$	$\left(\frac{c_{\mathrm{me}}}{c_{\mathrm{SiC}}}\right)_l$	$\left(\frac{c_{\mathrm{me}}}{c_{\mathrm{SiC}}}\right)_t$
SiC(FCC)	4.36	20.05	2.188	13035	6257	1	1	1	1
Si(FCC)	5.43	28.09	2.715	8470	5340	0.65	0.85	0.48	0.63
Al(FCC)	4.05	26.99	2.551	6360	3130	0.41	0.42	0.49	0.50
Ni(FCC)	3.52	58.71	2.218	5810	3080	1.25	1.38	0.45	0.49
Cu(FCC)	3.61	63.55	2.274	4760	2320	1.02	1.04	0.36	0.37
Ag(FCC)	4.09	107.87	2.576	3640	1690	0.92	0.89	0.28	0.27

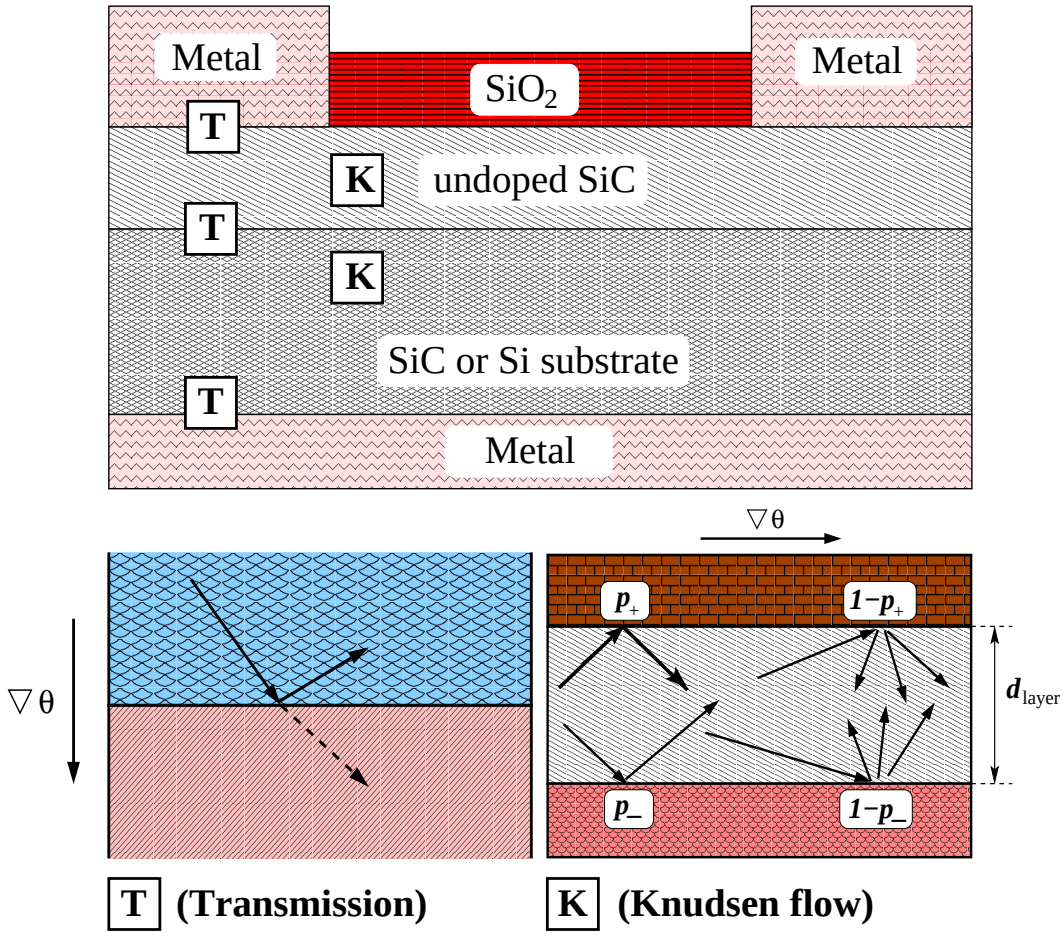

Figure 1: Structural schematics (top panel) and summary of key phonon transport effects (bottom panels) in a typical nanoscale SiC device. Oxide and substrate layers together with SiC/metal interfaces surrounds the thin (undoped) SiC transport channel. We find that heat dissipation is suppressed at room temperatures by the ineffective phonon transmission 'T' (lower left panel) across the SiC/metal or SiC/Si interfaces *and* by the phonon Knudsen effect 'K' (lower right panel), that is, the suppression of the thermal conductivity within the SiC by interface scattering at layer thicknesses $d_{\text{layer}} < 0.5$ μm. The phonon transport is calculated analytically at general probabilities, $p_{+(-)}$ and $1 - p_{+(-)}$, for specular and diffusive scattering at the upper (lower) interface.

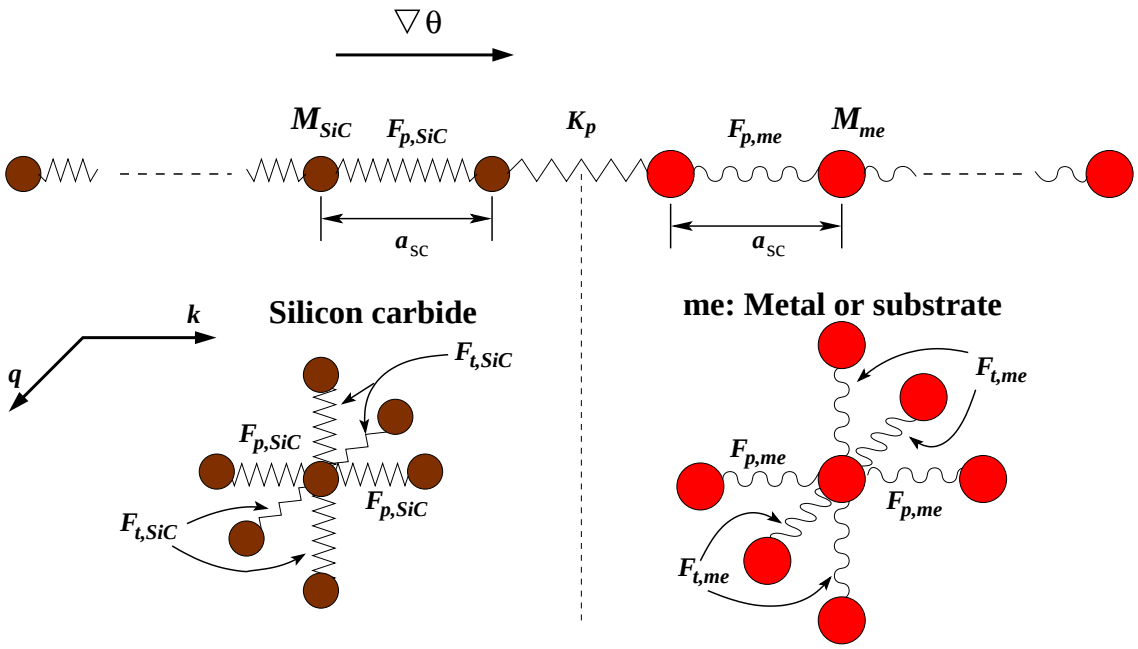

Figure 2: Schematics of the effective, atomistic representation in a simple-cubic (SC) model [2] adapted to estimate the finite-temperature phonon transport across SiC/metal (and SiC/Si) interface (vertical dashed line). The SC volume $a_{\rm sc}^3$ is chosen to contain exactly one physical atom but having the average atomic mass $M_{\rm SiC} = (M_{\rm Si} + M_{\rm C})/2$. A similar approach describes the neighboring media 'me' (metal or Si substrate). Force constants, $F_{p,t;\,{\rm SiC\,(me)}}$ fitted to the longitudinal and transverse sound velocities [2, 3], link the SC volumes within the SiC (metal) while elastic coupling constants $K_{p,t} \equiv \sqrt{F_{p,t;\,{\rm SiC}} F_{p,t;\,{\rm me}}}$ connect across the interface [3].

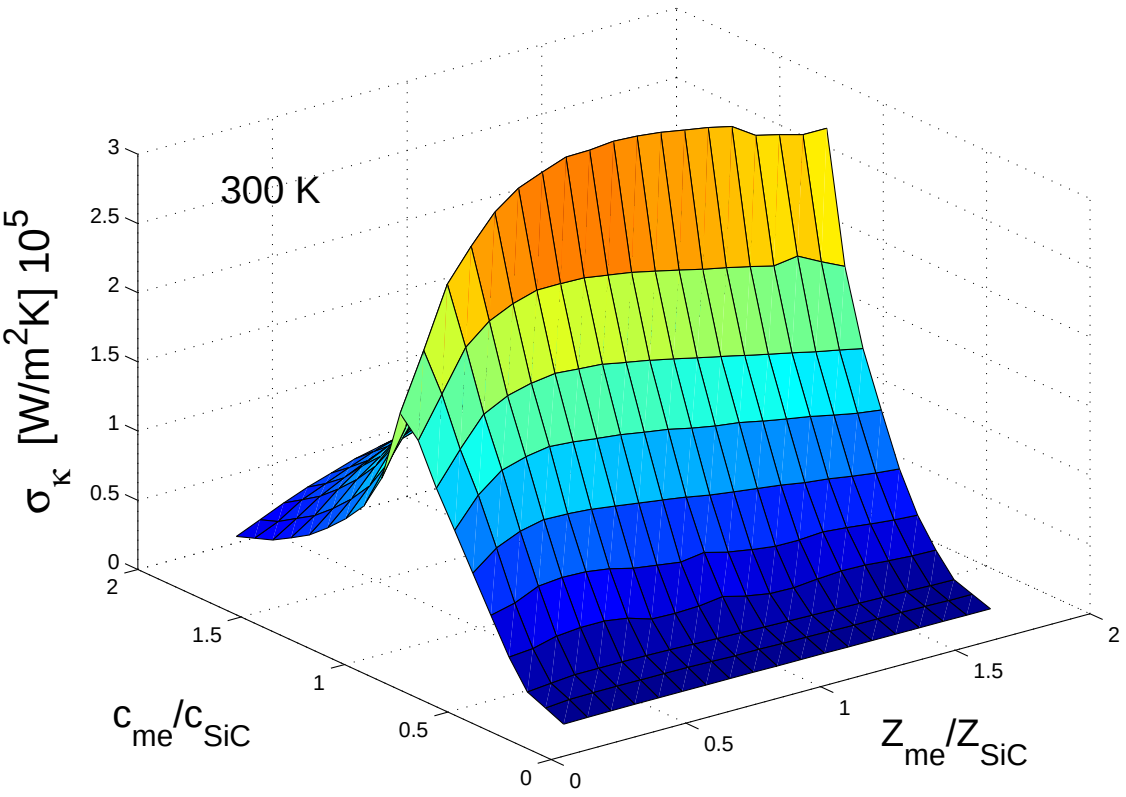

Figure 3: Dramatic variation of the room-temperature thermal conductance σ_K across a SiC/general-media interface specified by key differences in materials properties. A strong (weaker) dependence arises with the variation in the ratio of material sound velocities c (acoustic impedance Z) which specifies the amount of total internal phonon reflection (long-wavelength tunneling probability).

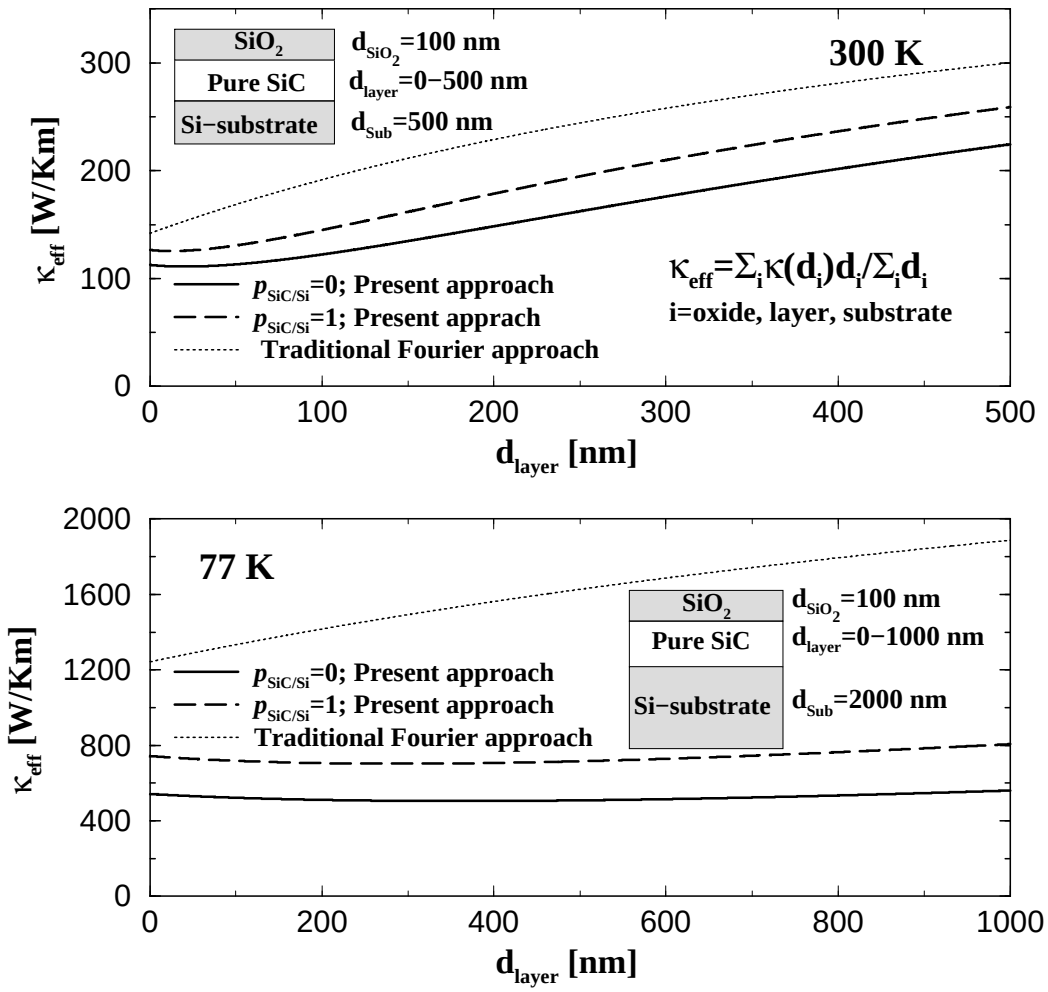

Figure 4: Knudsen suppression of the effective in-plane SiC transport $\kappa_{\rm eff}$ by interface scattering in the typical layered structures (inserts). The upper (lower) panel reports the variation with the thickness $d_{\rm layer}$ of SiC conductance channel at room (liquid-nitrogen) temperatures assuming either diffusive (solid curves) or specular (dashed curves) scattering at the SiC/Si-substrate interface. The traditional approach based on the Fourier law of heat flow (dotted curves) is documented to be inadequate due to the micron-scale phonon mean-free path.